



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:23 PM UTC

PDB ID : 6XTF / pdb\_00006xtf  
Title : Crystal structure a Thioredoxin Reductase from *Gloeobacter violaceus* bound to its electron donor  
Authors : Buey, R.M.; Gonzalez-Holgado, G.; Fernandez-Justel, D.; Balsera, M.  
Deposited on : 2020-01-16  
Resolution : 2.23 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](mailto: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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

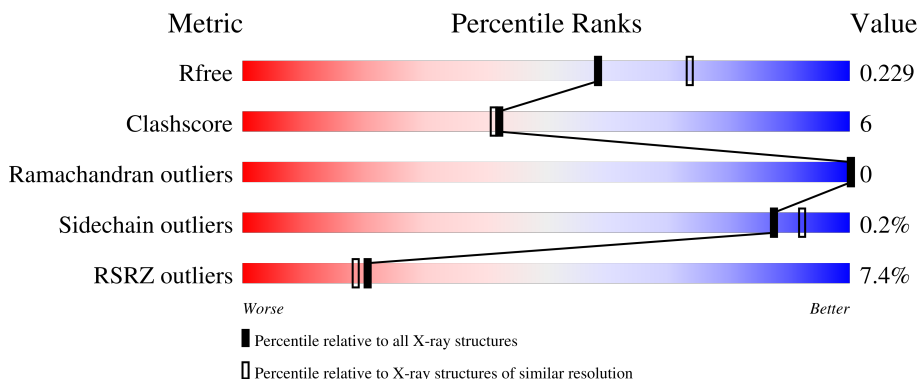
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.23 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (2.26-2.22)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	320	 5% 87% 12% .
1	B	320	 8% 88% 10% .
2	C	100	 5% 79% 17% .
2	D	100	 14% 75% 20% .

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	ACT	A	405	-	-	-	X

## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 13044 atoms, of which 6311 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 Thioredoxin reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
1	A	315	4729	1512	2352	412	441	12	0	1	0
1	B	315	4722	1508	2347	409	444	14	0	2	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q7NMP6
A	-1	SER	-	expression tag	UNP Q7NMP6
A	0	HIS	-	expression tag	UNP Q7NMP6
B	-2	GLY	-	expression tag	UNP Q7NMP6
B	-1	SER	-	expression tag	UNP Q7NMP6
B	0	HIS	-	expression tag	UNP Q7NMP6

- Molecule 2 is a protein called Ferredoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
2	C	96	1390	442	674	114	153	7	0	0	0
2	D	96	1340	432	639	111	151	7	0	0	0

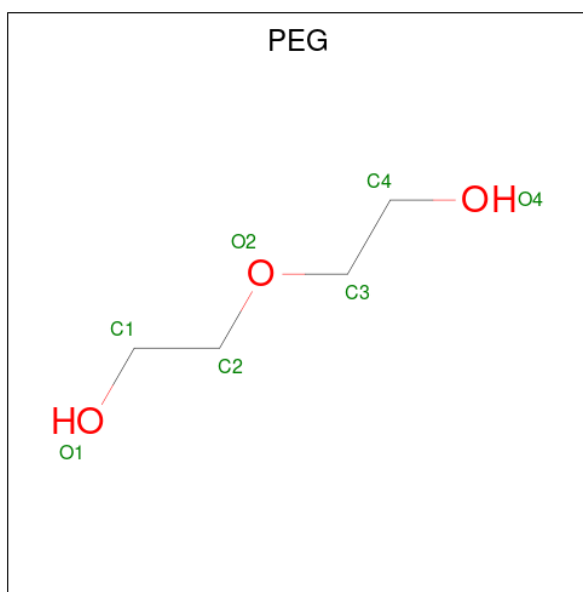
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP Q7NFA3
C	-1	SER	-	expression tag	UNP Q7NFA3
C	0	HIS	-	expression tag	UNP Q7NFA3
D	-2	GLY	-	expression tag	UNP Q7NFA3
D	-1	SER	-	expression tag	UNP Q7NFA3
D	0	HIS	-	expression tag	UNP Q7NFA3



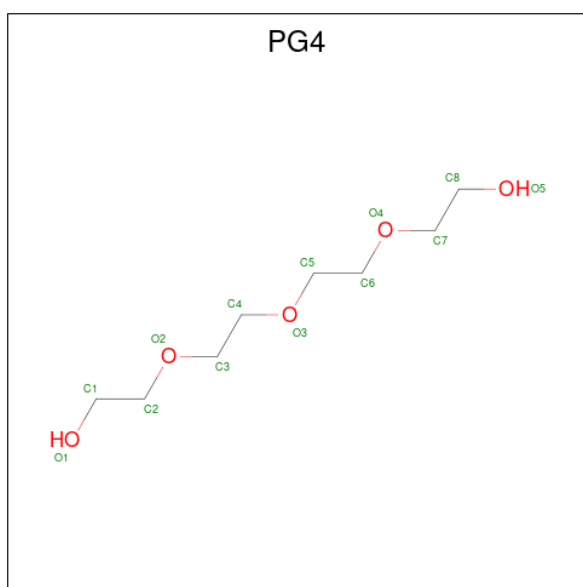
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	A	1	Total	C	H	O	0	0
			7	2	3	2		
4	B	1	Total	C	H	O	0	0
			7	2	3	2		
4	B	1	Total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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



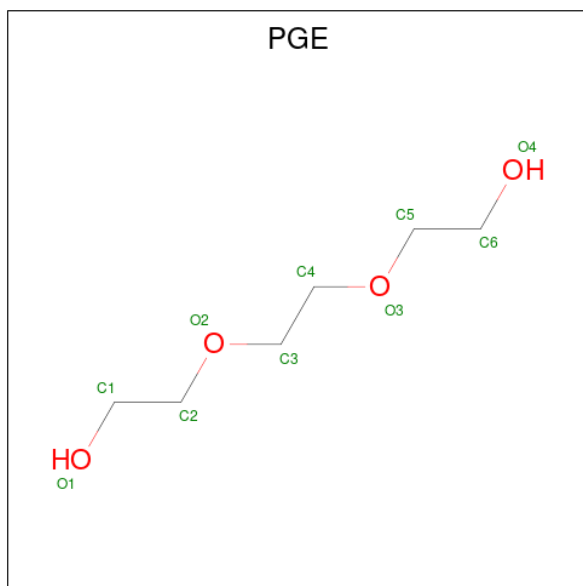
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	B	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>) (labeled as "Ligand of Interest" by depositor).



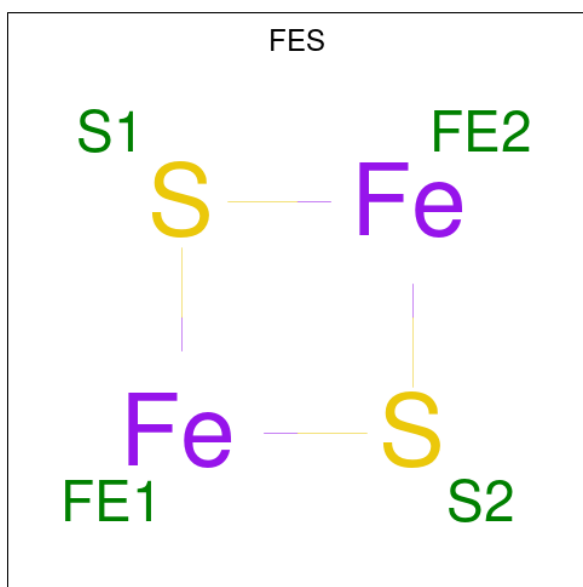
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	H	O	0	0
			31	8	18	5		
6	B	1	Total	C	H	O	0	0
			31	8	18	5		
6	B	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	H	O	0	0
			23	6	13	4		
7	A	1	Total	C	H	O	0	0
			23	6	13	4		
7	B	1	Total	C	H	O	0	0
			23	6	13	4		

- Molecule 8 is FE<sub>2</sub>/S<sub>2</sub> (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	Fe	S	0	0
			4	2	2		
8	D	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	94	Total	O	0	0
			94	94		
9	B	98	Total	O	0	0
			98	98		
9	C	46	Total	O	0	0
			46	46		
9	D	18	Total	O	0	0
			18	18		



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.74Å 181.31Å 80.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.37 – 2.23 83.37 – 2.23	Depositor EDS
% Data completeness (in resolution range)	67.0 (83.37-2.23) 67.1 (83.37-2.23)	Depositor EDS
$R_{merge}$	0.30	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.79 (at 2.22Å)	Xtrriage
Refinement program	PHENIX dev_3689	Depositor
R, $R_{free}$	0.201 , 0.232 0.200 , 0.229	Depositor DCC
$R_{free}$ test set	2035 reflections (3.40%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtrriage
Anisotropy	0.063	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 54.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	13044	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PEG, ACT, PG4, PGE, FAD, FES

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	0/2434	0.65	0/3311
1	B	0.47	1/2433 (0.0%)	0.77	5/3308 (0.2%)
2	C	0.36	0/727	0.64	0/987
2	D	0.41	0/712	0.89	2/970 (0.2%)
All	All	0.40	1/6306 (0.0%)	0.73	7/8576 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	270	VAL	CA-C	10.99	1.61	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	270	VAL	O-C-N	7.84	127.58	121.46
1	B	27	SER	CA-C-N	7.24	132.72	122.08
1	B	27	SER	C-N-CA	7.24	132.72	122.08
2	D	86	CYS	CA-C-N	6.59	132.82	122.94
2	D	86	CYS	C-N-CA	6.59	132.82	122.94
1	B	125	ALA	CA-C-N	-5.03	112.66	120.31
1	B	125	ALA	C-N-CA	-5.03	112.66	120.31

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2377	2352	2352	28	3
1	B	2375	2347	2347	24	1
2	C	716	674	673	14	0
2	D	701	639	638	16	2
3	A	53	30	31	0	0
3	B	53	30	31	3	0
4	A	28	21	21	0	0
4	B	16	12	12	1	0
4	D	4	3	3	0	0
5	A	21	30	30	5	0
5	B	21	30	30	2	0
5	C	28	40	40	3	0
5	D	7	10	10	0	0
6	A	13	18	18	0	0
6	B	26	36	36	3	0
7	A	20	26	28	1	0
7	B	10	13	14	0	0
8	C	4	0	0	1	0
8	D	4	0	0	1	0
9	A	94	0	0	1	0
9	B	98	0	0	6	0
9	C	46	0	0	0	0
9	D	18	0	0	1	0
All	All	6733	6311	6314	81	3

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 6.

All (81) 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:70:ASP:OD2	5:A:414:PEG:H12	1.64	0.96
1:A:70:ASP:OD2	5:A:414:PEG:C1	2.26	0.83
2:D:91:HIS:NE2	9:D:5301:HOH:O	2.22	0.72
6:B:405:PG4:O2	6:B:405:PG4:O5	2.08	0.71
3:B:401:FAD:H3B	9:B:505:HOH:O	1.93	0.69
1:A:5:ASP:HA	1:A:104:THR:OG1	1.93	0.68
2:D:54:SER:HB3	2:D:87:SER:HB2	1.76	0.67
6:B:405:PG4:O5	6:B:405:PG4:O3	2.12	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58:GLU:HA	9:B:507:HOH:O	1.96	0.65
2:C:62:GLN:OE1	2:C:65:LEU:N	2.29	0.64
1:B:117:ARG:HD3	1:B:238:LEU:HB2	1.80	0.64
1:A:183:ASP:O	1:A:183:ASP:OD1	2.16	0.63
1:B:117:ARG:HB3	1:B:117:ARG:NH2	2.13	0.63
2:D:5:LYS:HD2	2:D:18:ASP:OD1	1.98	0.63
1:B:177:LYS:HD3	2:D:27:ASP:OD2	1.99	0.62
2:C:23:GLU:OE1	2:C:31:ARG:NH1	2.33	0.62
1:A:135:CYS:SG	1:A:138:CYS:HB2	2.42	0.59
1:A:253:GLU:OE2	7:A:409:PGE:H4	2.03	0.59
1:B:117:ARG:HB3	1:B:117:ARG:HH21	1.68	0.58
3:B:401:FAD:C3B	9:B:505:HOH:O	2.53	0.56
2:C:53:VAL:CG2	2:C:89:GLU:HG3	2.36	0.56
2:D:54:SER:HB3	2:D:87:SER:CB	2.35	0.55
1:A:202:ARG:NH1	2:C:61:ASP:OD1	2.39	0.55
1:B:26:ARG:HH22	1:B:317:HIS:C	2.13	0.54
1:B:80:ARG:NH1	9:B:515:HOH:O	2.39	0.54
1:B:135[B]:CYS:SG	1:B:138[B]:CYS:HB2	2.48	0.54
1:A:202:ARG:NH2	2:C:58:ASP:OD2	2.41	0.53
1:A:221:PRO:HB2	2:C:22:ASP:HA	1.91	0.53
1:A:267:GLN:OE1	1:A:271:PRO:HA	2.09	0.53
1:B:112:THR:O	1:B:244:ILE:HD12	2.09	0.52
1:B:201:THR:HG22	1:B:220:HIS:CE1	2.45	0.52
2:D:62:GLN:OE1	2:D:65:LEU:N	2.33	0.52
1:B:244:ILE:HG23	5:B:410:PEG:H41	1.91	0.52
3:B:401:FAD:HM72	2:D:39:SER:HB3	1.92	0.51
2:C:68:ASP:HB3	5:C:105:PEG:H12	1.91	0.51
2:D:36:LEU:HB3	2:D:37:PRO:HD2	1.92	0.51
2:D:76:LEU:HD13	8:D:5202:FES:S2	2.50	0.50
1:A:59:MET:HE1	1:A:63[A]:HIS:CE1	2.47	0.50
1:A:106:ARG:HB3	5:A:407:PEG:H21	1.95	0.49
1:B:203:LEU:C	1:B:203:LEU:HD12	2.38	0.48
2:D:53:VAL:HB	2:D:87:SER:HB3	1.95	0.48
1:B:246:ASP:HB2	5:B:410:PEG:H32	1.95	0.48
2:D:5:LYS:CD	2:D:18:ASP:OD1	2.62	0.47
2:C:5:LYS:HE2	2:C:18:ASP:OD1	2.15	0.47
1:B:117:ARG:HD3	1:B:238:LEU:CB	2.43	0.47
2:D:52:MET:HE1	2:D:88:ILE:HG12	1.96	0.47
2:D:6:VAL:HA	2:D:86:CYS:O	2.15	0.46
1:A:74:GLU:OE2	5:A:414:PEG:H41	2.15	0.46
1:A:175:THR:OG1	1:A:199:GLU:HA	2.16	0.45

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:GLU:O	1:B:201:THR:HG23	2.16	0.45
1:B:48:LYS:HD2	1:B:58:GLU:OE1	2.16	0.45
4:B:411:ACT:OXT	9:B:501:HOH:O	2.21	0.45
1:A:223:GLU:O	1:A:224:SER:HB3	2.17	0.44
1:A:220:HIS:NE2	2:C:22:ASP:OD2	2.45	0.44
1:B:267:GLN:NE2	1:B:271:PRO:HA	2.32	0.44
1:A:158:VAL:O	1:A:162:GLN:HG3	2.17	0.44
1:A:245:THR:HB	1:A:254:MET:CE	2.48	0.44
2:C:76:LEU:HD13	8:C:101:FES:S2	2.58	0.43
1:A:95:LYS:HE2	5:A:403:PEG:O1	2.18	0.43
1:A:297:ALA:O	1:A:301:ILE:HG13	2.18	0.43
1:B:196:LYS:NZ	9:B:522:HOH:O	2.52	0.43
1:B:255:LYS:HE3	1:B:255:LYS:HB2	1.88	0.42
2:C:67:ASP:OD1	5:C:104:PEG:H22	2.19	0.42
1:B:145:ASN:C	1:B:169:SER:OG	2.62	0.42
2:C:25:ILE:HG12	2:C:80:ALA:O	2.19	0.42
2:D:25:ILE:HG12	2:D:80:ALA:O	2.18	0.42
1:A:66:GLU:HG3	1:B:192:HIS:CD2	2.54	0.42
2:D:51:LYS:HE2	2:D:51:LYS:HB3	1.87	0.42
1:A:202:ARG:HH22	2:C:58:ASP:CG	2.28	0.42
1:B:128:LEU:CD1	1:B:134:TYR:CE2	3.03	0.41
6:B:402:PG4:O1	6:B:402:PG4:O4	2.38	0.41
1:A:280:ARG:NH2	9:A:508:HOH:O	2.44	0.41
1:A:178:ASP:O	1:A:181:THR:OG1	2.37	0.41
1:A:245:THR:HB	1:A:254:MET:HE1	2.01	0.41
1:B:265:MET:SD	1:B:303:ARG:NH2	2.93	0.41
1:B:295:CYS:O	1:B:299:MET:HG3	2.21	0.41
1:A:45:ILE:CD1	1:A:115:MET:HE2	2.52	0.40
2:D:87:SER:C	2:D:88:ILE:HG13	2.45	0.40
1:A:91:GLU:HB3	1:A:92:PRO:HD2	2.04	0.40
2:C:35:ASP:OD1	5:C:103:PEG:H11	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ASP:H	1:B:286:GLN:HE22[6_445]	1.23	0.37
1:A:308:ARG:HH12	2:D:94:ASP:OD1[6_445]	1.26	0.34
1:A:308:ARG:NH1	2:D:94:ASP:OD1[6_445]	2.07	0.13

## 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	314/320 (98%)	306 (98%)	8 (2%)	0	100	100
1	B	315/320 (98%)	308 (98%)	7 (2%)	0	100	100
2	C	94/100 (94%)	88 (94%)	6 (6%)	0	100	100
2	D	94/100 (94%)	89 (95%)	5 (5%)	0	100	100
All	All	817/840 (97%)	791 (97%)	26 (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	244/252 (97%)	244 (100%)	0	100	100
1	B	245/252 (97%)	244 (100%)	1 (0%)	84	88
2	C	79/83 (95%)	79 (100%)	0	100	100
2	D	75/83 (90%)	75 (100%)	0	100	100
All	All	643/670 (96%)	642 (100%)	1 (0%)	87	92

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	203	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	B	227	GLN
1	B	267	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](#)

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

33 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	A	406	-	12,12,12	0.54	0	11,11,11	0.27	0
5	PEG	C	103	-	6,6,6	0.51	0	5,5,5	0.20	0
4	ACT	A	404	-	3,3,3	1.21	0	3,3,3	1.28	0
3	FAD	A	401	-	58,58,58	0.36	0	85,89,89	0.37	0
8	FES	D	5202	2	0,4,4	-	-	-		
4	ACT	B	406	-	3,3,3	1.25	0	3,3,3	1.39	0
4	ACT	B	407	-	3,3,3	1.26	0	3,3,3	1.40	0
4	ACT	A	412	-	3,3,3	1.35	0	3,3,3	1.44	0
5	PEG	B	403	-	6,6,6	0.49	0	5,5,5	0.18	0
4	ACT	A	405	-	3,3,3	1.24	0	3,3,3	1.31	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	PEG	A	414	-	6,6,6	0.56	0	5,5,5	0.39	0
5	PEG	C	105	-	6,6,6	0.52	0	5,5,5	0.16	0
6	PG4	B	405	-	12,12,12	0.77	0	11,11,11	0.39	0
4	ACT	D	5201	-	3,3,3	1.28	0	3,3,3	1.28	0
6	PG4	B	402	-	12,12,12	0.54	0	11,11,11	0.38	0
3	FAD	B	401	-	58,58,58	0.38	0	85,89,89	0.39	0
5	PEG	C	104	-	6,6,6	0.49	0	5,5,5	0.20	0
5	PEG	D	5203	-	6,6,6	0.50	0	5,5,5	0.19	0
7	PGE	A	409	-	9,9,9	0.47	0	8,8,8	0.22	0
5	PEG	A	403	-	6,6,6	0.50	0	5,5,5	0.13	0
5	PEG	B	410	-	6,6,6	0.51	0	5,5,5	0.36	0
5	PEG	A	407	-	6,6,6	0.50	0	5,5,5	0.17	0
8	FES	C	101	2	0,4,4	-	-	-	-	-
7	PGE	B	409	-	9,9,9	0.53	0	8,8,8	0.21	0
4	ACT	A	413	-	3,3,3	0.90	0	3,3,3	1.23	0
4	ACT	B	404	-	3,3,3	1.17	0	3,3,3	1.33	0
4	ACT	A	411	-	3,3,3	1.09	0	3,3,3	1.46	0
4	ACT	A	402	-	3,3,3	1.06	0	3,3,3	1.31	0
5	PEG	B	408	-	6,6,6	0.51	0	5,5,5	0.19	0
4	ACT	B	411	-	3,3,3	1.27	0	3,3,3	1.43	0
4	ACT	A	410	-	3,3,3	1.23	0	3,3,3	1.41	0
5	PEG	C	102	-	6,6,6	0.50	0	5,5,5	0.11	0
7	PGE	A	408	-	9,9,9	0.54	0	8,8,8	0.25	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PG4	A	406	-	-	8/10/10/10	-
5	PEG	C	103	-	-	2/4/4/4	-
8	FES	D	5202	2	-	-	0/1/1/1
3	FAD	A	401	-	-	0/34/50/50	0/6/6/6
5	PEG	B	403	-	-	2/4/4/4	-
5	PEG	A	414	-	-	2/4/4/4	-
5	PEG	C	105	-	-	3/4/4/4	-
6	PG4	B	405	-	-	2/10/10/10	-
6	PG4	B	402	-	-	7/10/10/10	-
3	FAD	B	401	-	-	1/34/50/50	0/6/6/6
5	PEG	C	104	-	-	3/4/4/4	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	D	5203	-	-	2/4/4/4	-
7	PGE	A	409	-	-	3/7/7/7	-
5	PEG	A	403	-	-	1/4/4/4	-
5	PEG	B	410	-	-	3/4/4/4	-
5	PEG	A	407	-	-	2/4/4/4	-
8	FES	C	101	2	-	-	0/1/1/1
7	PGE	B	409	-	-	1/7/7/7	-
5	PEG	B	408	-	-	3/4/4/4	-
5	PEG	C	102	-	-	3/4/4/4	-
7	PGE	A	408	-	-	5/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	409	PGE	O2-C3-C4-O3
6	A	406	PG4	O3-C5-C6-O4
5	A	414	PEG	O1-C1-C2-O2
6	A	406	PG4	O4-C7-C8-O5
6	B	402	PG4	O3-C5-C6-O4
5	A	407	PEG	O1-C1-C2-O2
5	A	407	PEG	O2-C3-C4-O4
5	C	104	PEG	O1-C1-C2-O2
5	C	105	PEG	O2-C3-C4-O4
7	A	409	PGE	O3-C5-C6-O4
5	B	403	PEG	O2-C3-C4-O4
5	B	408	PEG	O1-C1-C2-O2
7	A	408	PGE	O1-C1-C2-O2
7	A	408	PGE	O2-C3-C4-O3
5	B	410	PEG	O1-C1-C2-O2
5	C	104	PEG	O2-C3-C4-O4
5	D	5203	PEG	O2-C3-C4-O4
5	C	105	PEG	O1-C1-C2-O2
5	D	5203	PEG	O1-C1-C2-O2
6	A	406	PG4	O1-C1-C2-O2
5	C	102	PEG	O1-C1-C2-O2
7	A	408	PGE	O3-C5-C6-O4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
5	A	403	PEG	O1-C1-C2-O2
6	B	402	PG4	C4-C3-O2-C2
6	B	402	PG4	C1-C2-O2-C3
3	B	401	FAD	PA-O3P-P-O5'
5	C	103	PEG	C4-C3-O2-C2
6	A	406	PG4	C5-C6-O4-C7
6	A	406	PG4	C4-C3-O2-C2
7	A	408	PGE	C3-C4-O3-C5
5	C	102	PEG	C1-C2-O2-C3
5	B	408	PEG	O2-C3-C4-O4
6	B	405	PG4	O2-C3-C4-O3
5	B	403	PEG	C1-C2-O2-C3
6	A	406	PG4	C1-C2-O2-C3
6	A	406	PG4	O2-C3-C4-O3
7	A	409	PGE	C6-C5-O3-C4
5	B	410	PEG	C1-C2-O2-C3
5	C	103	PEG	C1-C2-O2-C3
5	A	414	PEG	O2-C3-C4-O4
5	C	102	PEG	O2-C3-C4-O4
7	A	408	PGE	C4-C3-O2-C2
6	B	402	PG4	O4-C7-C8-O5
6	B	402	PG4	C5-C6-O4-C7
5	B	408	PEG	C4-C3-O2-C2
6	A	406	PG4	C8-C7-O4-C6
5	B	410	PEG	C4-C3-O2-C2
7	B	409	PGE	C6-C5-O3-C4
5	C	104	PEG	C4-C3-O2-C2
5	C	105	PEG	C4-C3-O2-C2
6	B	402	PG4	O2-C3-C4-O3
6	B	405	PG4	C1-C2-O2-C3
6	B	402	PG4	O1-C1-C2-O2

There are no ring outliers.

14 monomers are involved in 20 short contacts:

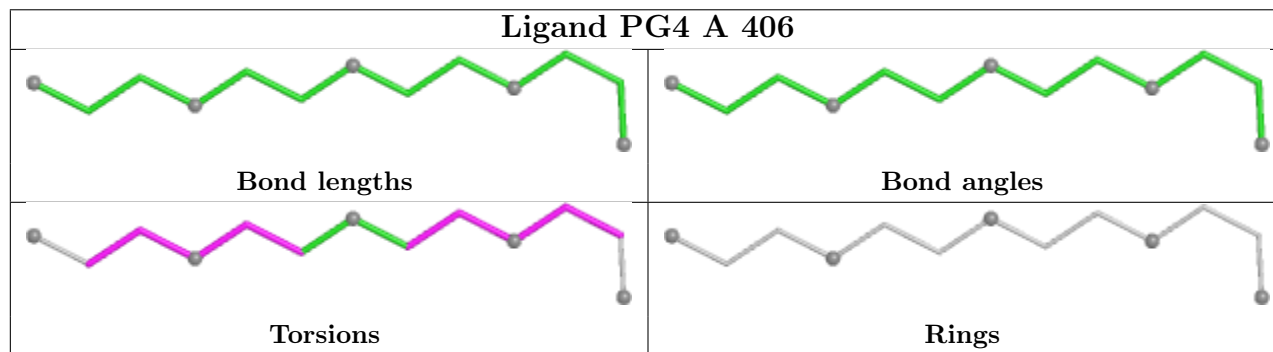
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	103	PEG	1	0
8	D	5202	FES	1	0
5	A	414	PEG	3	0
5	C	105	PEG	1	0
6	B	405	PG4	2	0
6	B	402	PG4	1	0

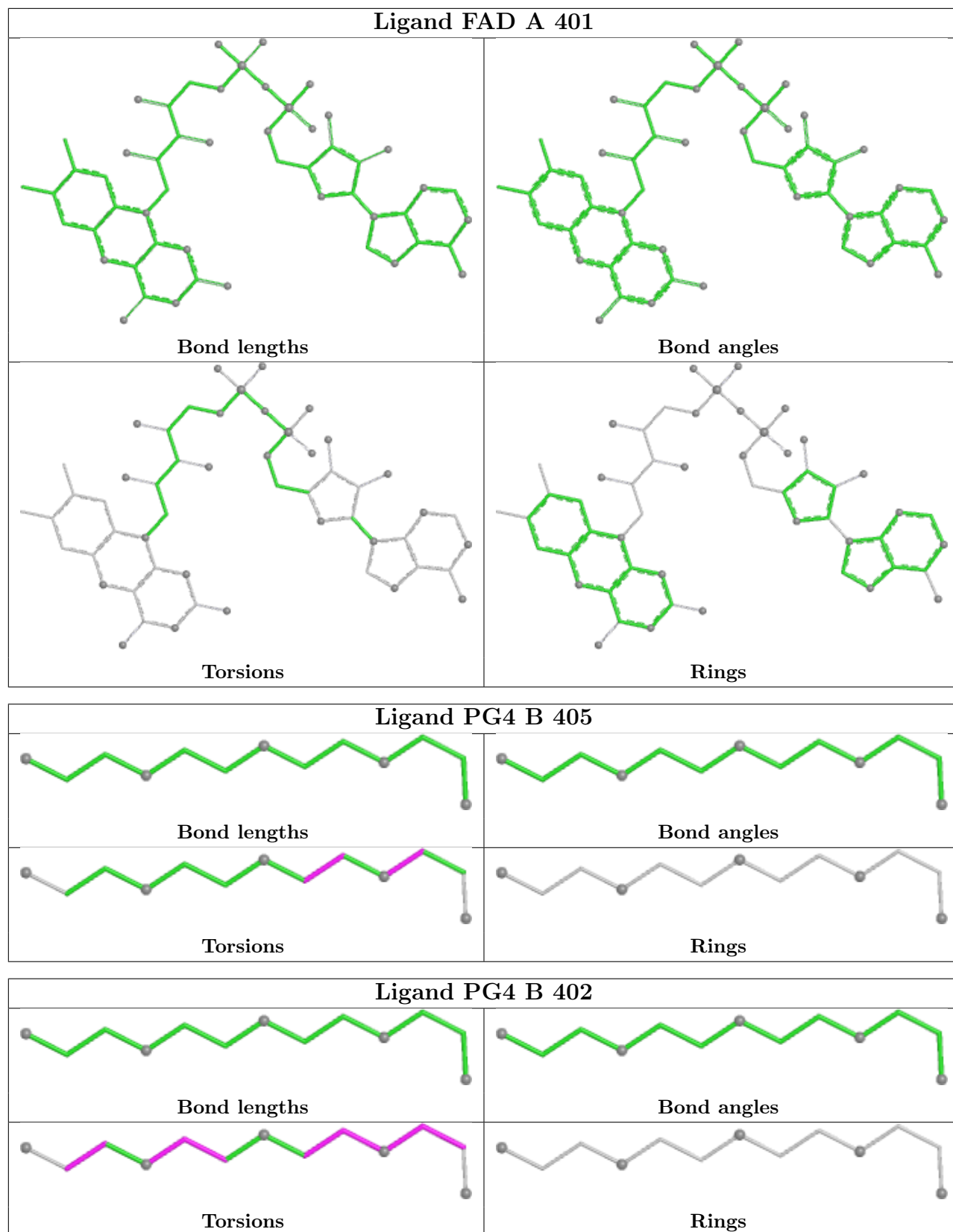
*Continued on next page...*

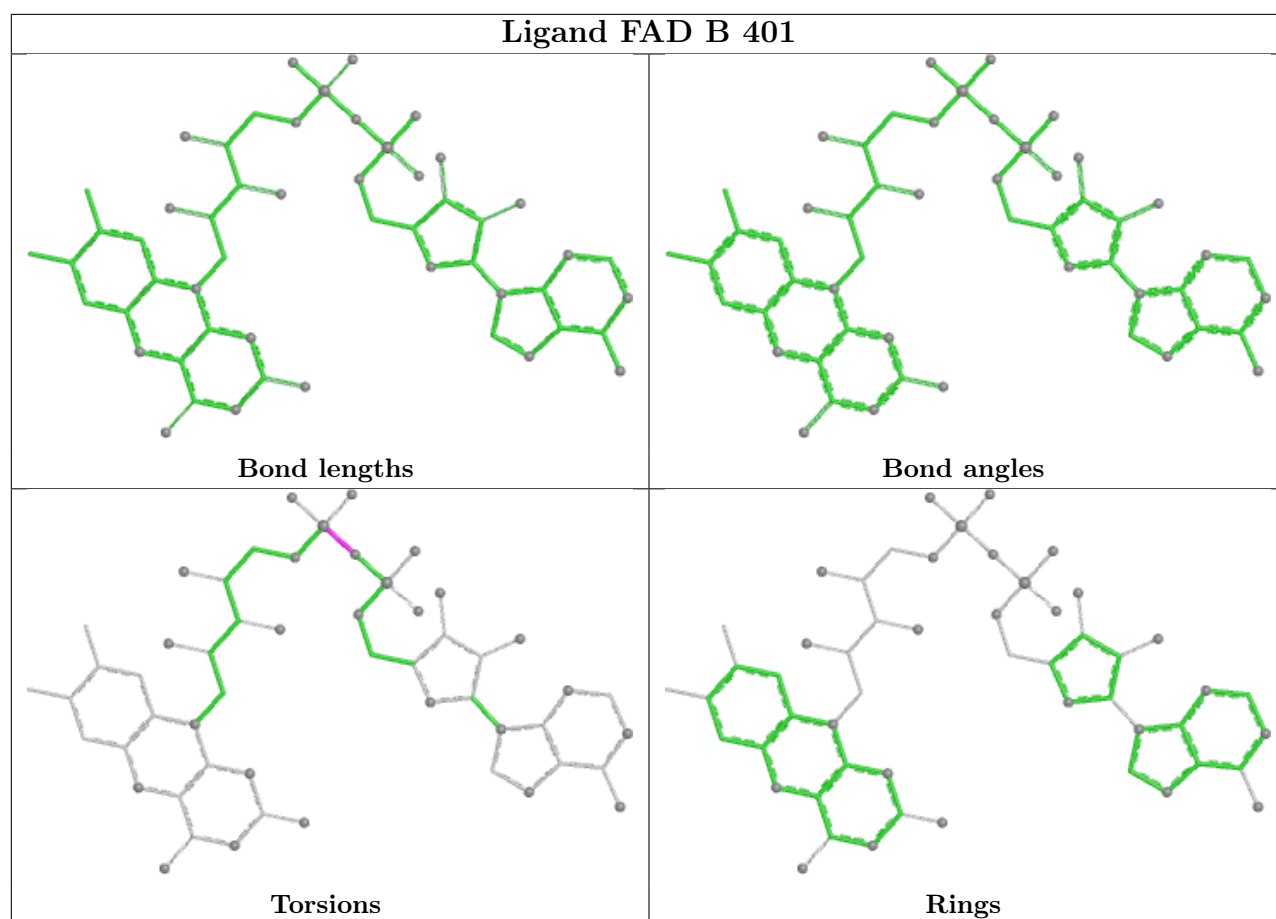
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	401	FAD	3	0
5	C	104	PEG	1	0
7	A	409	PGE	1	0
5	A	403	PEG	1	0
5	B	410	PEG	2	0
5	A	407	PEG	1	0
8	C	101	FES	1	0
4	B	411	ACT	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 than 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	315/320 (98%)	0.20	17 (5%) 31 29	12, 33, 66, 107	1 (0%)
1	B	315/320 (98%)	0.22	25 (7%) 18 16	18, 33, 71, 105	2 (0%)
2	C	96/100 (96%)	-0.02	5 (5%) 33 31	17, 31, 51, 81	0
2	D	96/100 (96%)	0.93	14 (14%) 6 5	31, 55, 84, 101	0
All	All	822/840 (97%)	0.27	61 (7%) 20 18	12, 35, 72, 107	3 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	317	HIS	7.3
1	A	174	ILE	6.3
1	B	265	MET	5.6
2	D	87	SER	4.6
1	A	268	THR	4.4
1	B	28	GLU	4.2
1	B	185	HIS	4.2
1	B	3	GLN	4.2
1	B	257	ASP	4.1
1	B	182	LEU	3.8
1	B	117	ARG	3.7
1	B	181	THR	3.7
1	B	317	HIS	3.5
1	B	211	ALA	3.5
1	B	5	ASP	3.5
1	B	4	PHE	3.4
1	A	138	CYS	3.4
1	B	180	HIS	3.3
1	B	264	GLU	3.3
1	A	47	HIS	3.1
2	D	36	LEU	3.1

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
2	D	31	ARG	3.0
2	D	35	ASP	3.0
2	C	79	VAL	3.0
2	D	34	LEU	3.0
1	A	223	GLU	3.0
2	D	8	LEU	2.9
1	A	183	ASP	2.9
1	B	253	GLU	2.9
1	A	316	ALA	2.8
1	B	217	GLU	2.8
1	B	126	GLU	2.7
2	D	2	ALA	2.7
2	C	35	ASP	2.7
2	D	18	ASP	2.7
1	B	210	GLU	2.7
1	B	118	ILE	2.7
1	B	58	GLU	2.6
1	A	293	ASP	2.6
2	D	68	ASP	2.6
1	B	179	PRO	2.6
1	B	90	SER	2.6
1	A	188	GLU	2.5
1	A	225	ASP	2.5
1	A	224	SER	2.5
1	B	142	PHE	2.5
1	A	28	GLU	2.5
2	D	3	THR	2.5
2	D	14	LYS	2.5
1	B	47	HIS	2.4
1	A	199	GLU	2.3
1	B	203	LEU	2.3
1	A	58	GLU	2.3
2	C	2	ALA	2.3
2	D	88	ILE	2.2
1	A	292	GLY	2.2
2	C	44	ALA	2.2
2	D	5	LYS	2.2
1	A	77	THR	2.1
2	C	39	SER	2.1
2	D	12	SER	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

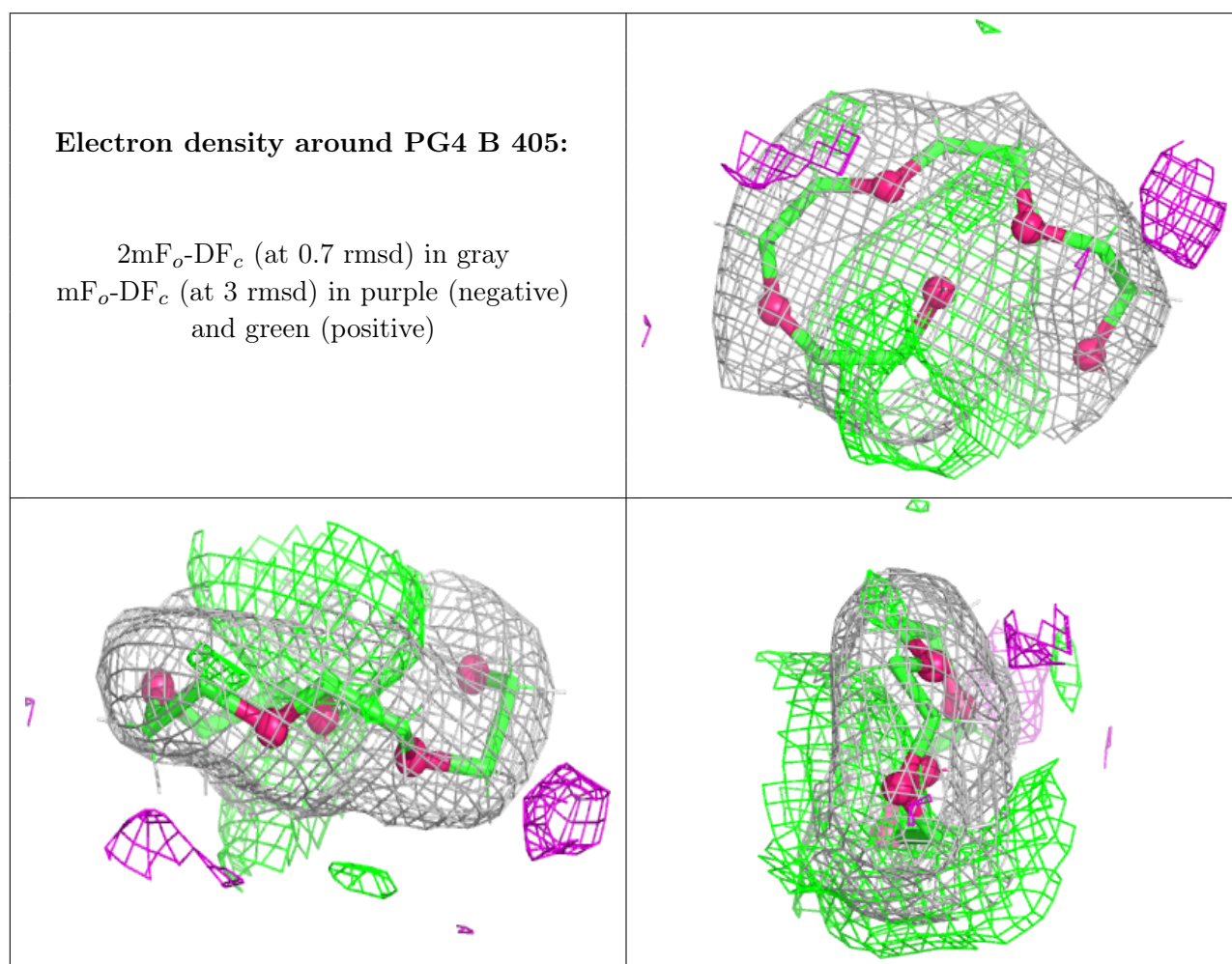
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ACT	D	5201	4/4	0.56	0.33	53,61,65,65	0
4	ACT	A	412	4/4	0.65	0.26	59,68,82,82	0
4	ACT	A	405	4/4	0.68	0.43	81,102,128,128	0
5	PEG	C	104	7/7	0.69	0.18	25,36,49,49	0
4	ACT	B	407	4/4	0.76	0.23	56,65,68,68	0
5	PEG	A	414	7/7	0.77	0.27	87,110,138,140	0
6	PG4	B	405	13/13	0.78	0.21	33,48,69,69	0
4	ACT	A	404	4/4	0.79	0.31	72,81,100,100	0
4	ACT	A	413	4/4	0.81	0.23	74,82,92,92	0
4	ACT	B	411	4/4	0.81	0.17	48,55,59,59	0
5	PEG	D	5203	7/7	0.82	0.21	53,69,91,91	0
5	PEG	B	403	7/7	0.82	0.15	42,54,66,66	0
7	PGE	A	409	10/10	0.82	0.28	70,106,130,134	0
4	ACT	B	406	4/4	0.83	0.19	41,51,55,65	0
4	ACT	B	404	4/4	0.84	0.17	46,57,68,68	0
5	PEG	A	403	7/7	0.84	0.19	52,71,91,91	0
6	PG4	B	402	13/13	0.85	0.18	49,74,91,92	0
4	ACT	A	402	4/4	0.87	0.25	60,64,87,87	0
5	PEG	B	408	7/7	0.88	0.23	86,104,117,118	0
4	ACT	A	411	4/4	0.88	0.20	48,54,66,66	0
7	PGE	A	408	10/10	0.89	0.26	80,109,134,135	0
5	PEG	A	407	7/7	0.90	0.19	64,78,91,91	0
5	PEG	B	410	7/7	0.90	0.20	21,48,85,85	0
5	PEG	C	103	7/7	0.90	0.15	57,70,89,89	0
5	PEG	C	105	7/7	0.91	0.13	39,48,58,58	0
6	PG4	A	406	13/13	0.91	0.14	32,54,77,77	0
7	PGE	B	409	10/10	0.91	0.21	95,115,123,125	0

*Continued on next page...*

Continued from previous page...

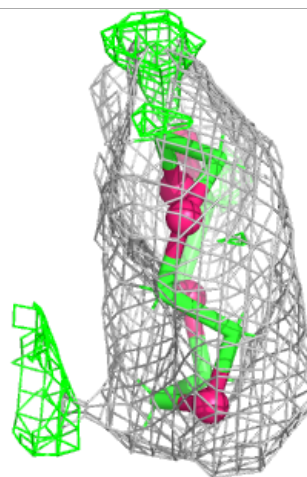
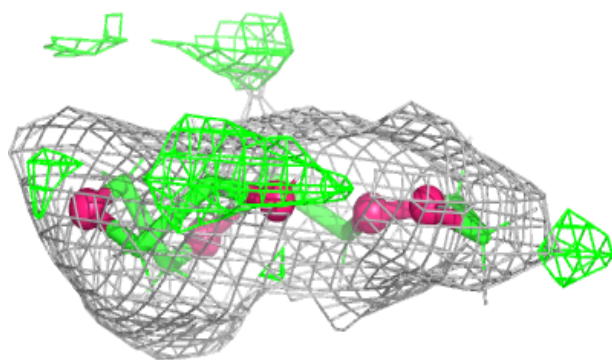
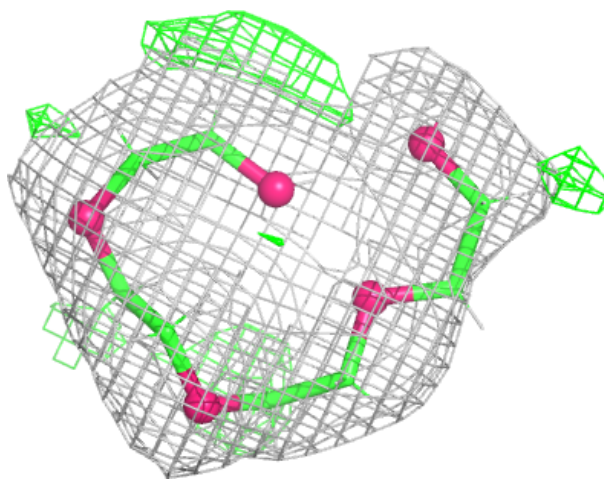
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	PEG	C	102	7/7	0.94	0.12	26,33,70,73	0
3	FAD	A	401	53/53	0.95	0.16	13,52,85,112	0
8	FES	D	5202	4/4	0.96	0.07	27,35,38,45	0
8	FES	C	101	4/4	0.97	0.07	24,26,32,38	0
4	ACT	A	410	4/4	0.97	0.13	11,20,34,39	0
3	FAD	B	401	53/53	0.98	0.06	8,23,34,42	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.



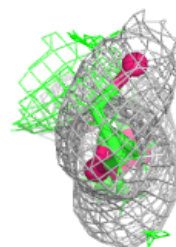
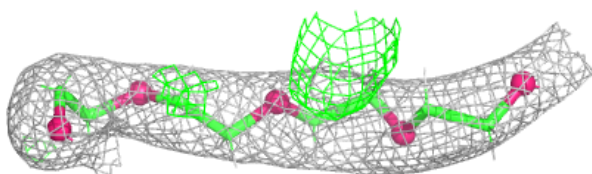
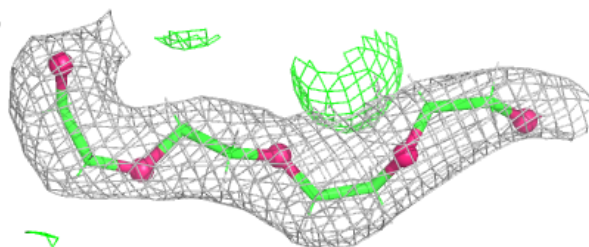
**Electron density around PG4 B 402:**

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

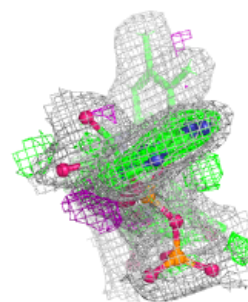
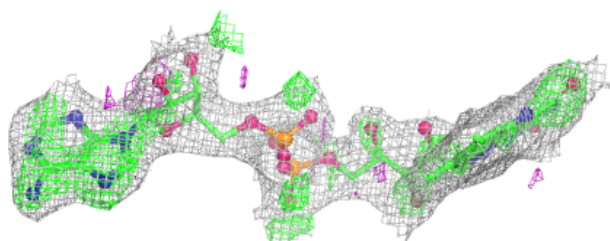
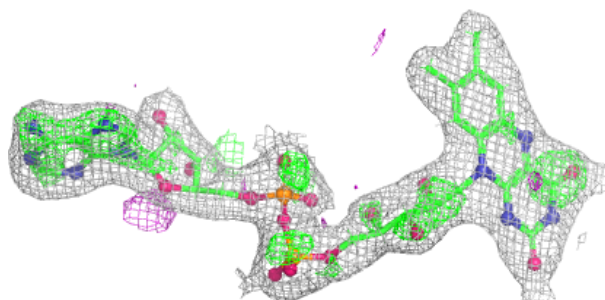


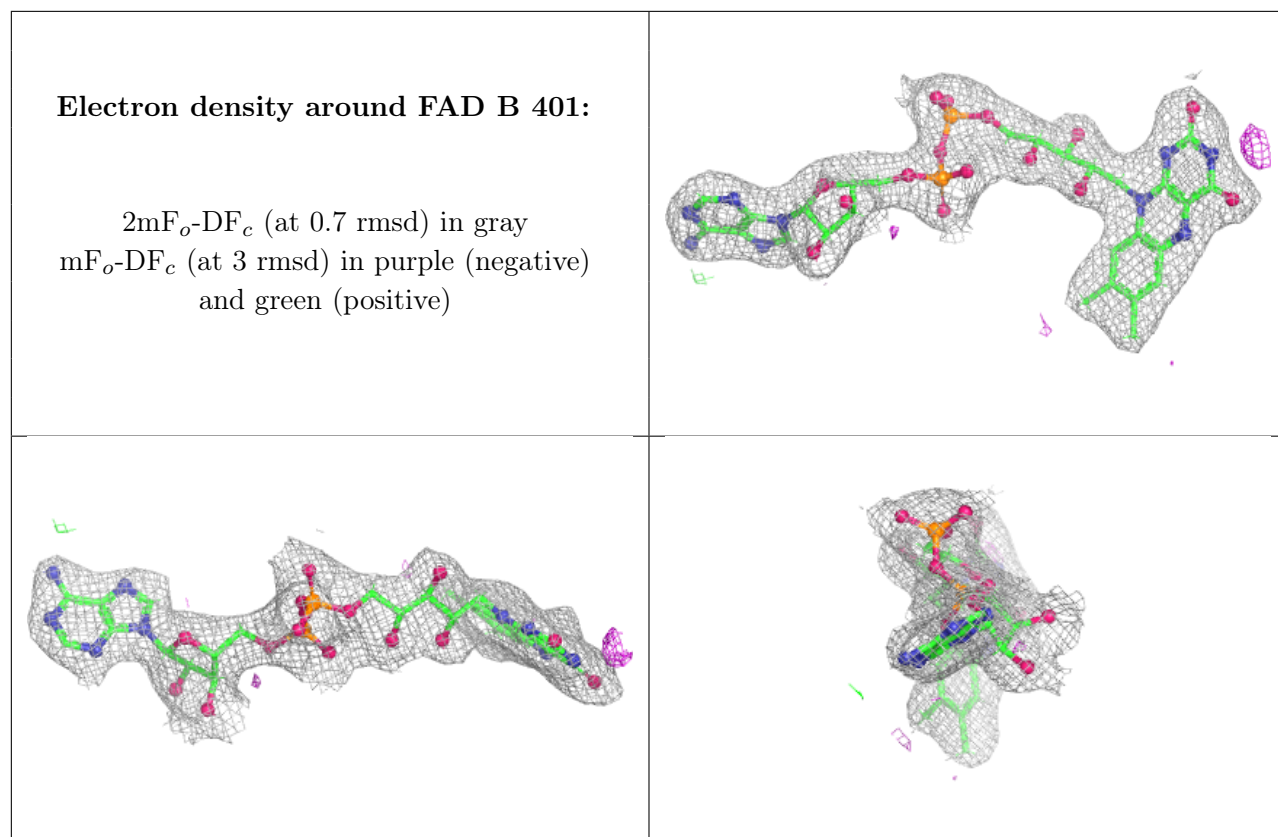
**Electron density around PG4 A 406:**

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

**Electron density around FAD A 401:**

$2mF_o-DF_c$  (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.